Quantum Chemistry Calculations using Energy Derivatives on Quantum Computers

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SUMMARY

Quantum chemistry is one area that is speculated to benefit the most from the development of quantum computers. For this purpose, variational algorithms like variational quantum eigensolver (VQE) have been developed for near-term quantum hardware for determining various physical and chemical properties of a chemical system or a chemical reaction. Recent work in the field has primarily focused on developing the theory of VQE, and VQE-based algorithms for calculations of molecular ground-state energies [1], excited state energies [2], molecular vibrations [3], etc. This work presents a VQE-based method to calculate molecular energy derivatives with respect to system parameters on a quantum computer for ground state energy and excited state energies up to the second-order, which are important to calculate a range of time-independent physical and chemical properties such as minimum energy configuration, molecular response properties, etc.

MOTIVATION

Quantum chemistry calculations such as the prediction of molecular properties and modeling of chemical reactions are a few of the critical areas where near-term quantum computers can showcase quantum advantage. We present a method to calculate energy derivatives for both ground state and excited state energies with respect to the parameters of a chemical system based on the framework of the variational quantum eigensolver (VQE). A low-depth implementation of quantum circuits within the hybrid variational paradigm is designed, and their computational costs are analyzed. We showcase the effectiveness of our method by incorporating it in some key quantum chemistry applications of energy derivatives, such as to perform minimum energy configuration search and estimate molecular response properties estimation of H2 molecule, and also to find the transition state of H2 + H ↔ H + H2 reaction. The obtained results are shown to be in complete agreement with their respective full configuration interaction (FCI) values.

PROJECT DESCRIPTION

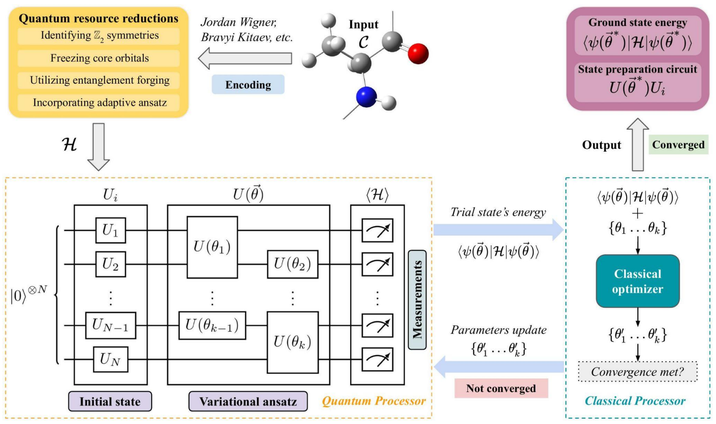
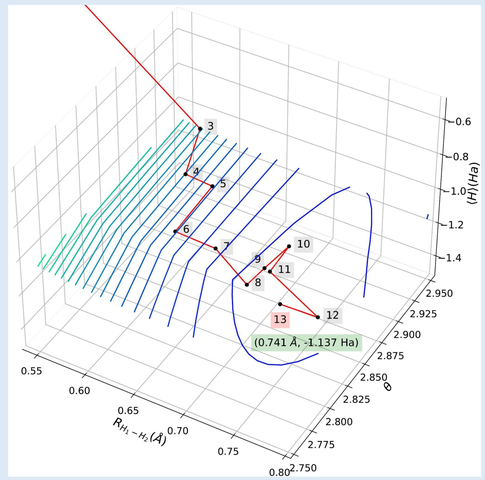


FIG. 1: Workflow for the variational quantum eigensolver

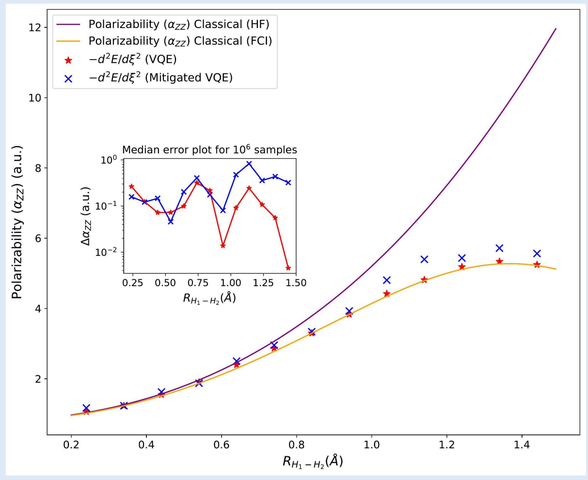
RESULTS

We show the use of these energy derivatives for the following quantum chemistry tasks: (i) minimum energy configuration search for H_2 molecule, (ii) estimation of molecular response properties such as dipole moment and polarizability for H2 molecule, and (iii) transition state search for the reaction $H_2 + H \leftrightarrow H + H_2$ (Fig. 2c). Our variational method gives results in complete agreement with those obtained using full configuration interaction (FCI) values. Additionally, we also show the first-order excited state energy derivatives for H2 molecule. The corresponding classical calculations and generation of Hamiltonian terms were done using PySCF, Gaussian and OpenFermion. Their derivatives $\partial\eta_i\hat{H}(\eta)$, and $\partial\eta_i\partial\eta_j\hat{H}(\eta)$ are calculated using central-differencing method with step-size 0.001. The experiments were performed using IBM Qiskit [5]. For noisy simulations, the noise data was taken from the IBMQ vigo backend [6], whereas Ignis and Mitiq [7] frameworks were used for software-level error mitigation.

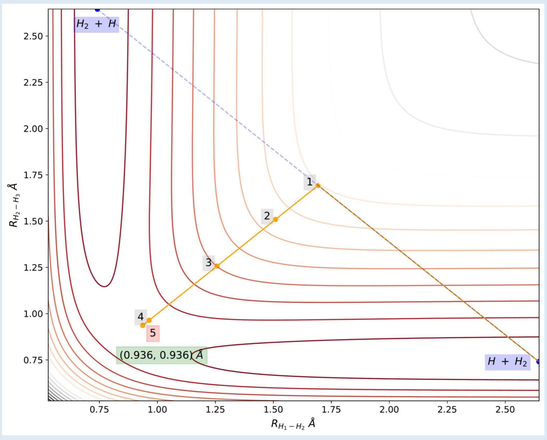
(a)



(b)



(c)



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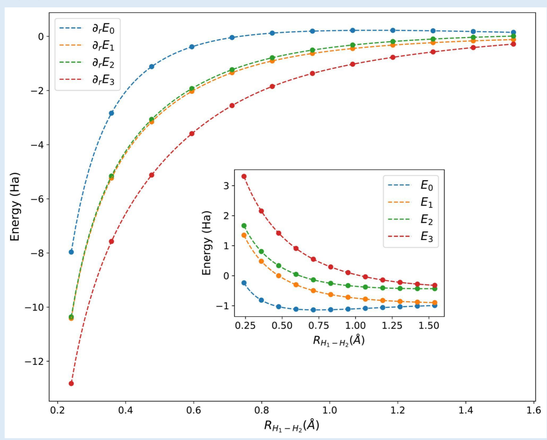

FIG 2. (a) Minimum energy configuration search for H_2 molecule using gradient descent method with first-order energy derivatives. (b) Molecular response property (here polarization) calculation for H_2 molecule. (c) Transition state search for the reaction $H + H_2 \leftrightarrow H_2 + H$. (d) Energy derivatives of ground state and excited energy states for H_2 molecule.

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